

Semiclassical theory of attosecond pulse generation

V.T. Platonenko, A.F. Sterjantov

Abstract. A numerical model is developed for calculating the single-atomic response to the field of a linearly polarised laser pulse of duration of a few oscillation cycles of the optical field. The model is based on the semiclassical theory of high-order harmonic generation and is developed in the time representation. The parameters of generated attosecond pulses calculated within the framework of the model are in good agreement with the results obtained by integrating numerically the Schrödinger equation. The complexity of model calculations is approximately two orders of magnitude lower than that of the numerical integration of the Schrödinger equation.

Keywords: attosecond pulses, high-order harmonics, radiative recombination, coherence, tunnel ionisation, Schrödinger levels, wave packet, numerical simulation.

1. Introduction

The generation of soft X-rays upon tunnel (or above-barrier) ionisation of atoms in the field of a light wave and the subsequent coherent radiative recombination (CRR) of electrons on parent ions is an efficient tool for producing coherent X-ray pulses with controllable parameters. In the case of monochromatic optical excitation, CRR is, in fact, the high-order harmonic generation (HOHG) [1, 2]. If excitation is performed by a laser pulse of duration of a few oscillation cycles of the optical field, it is possible to generate a single attosecond pulse (AP) – an X-ray pulse with a continuous spectrum and duration that is approximately an order of magnitude smaller than the cycle of the exciting field [3].

The observation and measurements of the AP parameters involves considerable difficulties. Therefore, the prediction of these parameters as accurately and detailed as possible by using the theoretical analysis and numerical calculations is of current interest. The parameters of fields

generated during CRR in an elementary volume of a medium are mainly determined by the interaction of the exciting field with a single atom, whereas the interaction between atoms is usually insignificant. Therefore, to control efficiently the AP parameters, it is important first of all to understand the generation mechanism of an AP by a single atom.

The most generally employed theoretical methods describing CRR were initially developed for the HOHG. The HOHG mechanism in gases is comparatively well described by the semiclassical Corcum theory [4]. The basic concepts of this theory can be extended to CRR in the field of a laser pulse of an arbitrary duration. In this case, CRR should be treated as a complex process including tunnel ionisation, the stage of the free motion of an electron in the light wave field, and the radiative recombination of an electron returning to the parent ion and undergoing the transition to the initial state. It is assumed that ionisation and recombination are instantaneous events, the velocity of the electron immediately after ionisation is zero, and the trajectory of the free electron begins and terminates near the parent ion and is determined by the classical equations of motion. The instantaneous frequency of light emitted at some instant of time (the sum of the ionisation energy and kinetic energy acquired during free motion) is unambiguously determined by the time dependence of the electric field. This simple one-electron model allows one to determine the maximum frequency of the field generated by an atom (the cut-off frequency) and clearly illustrates the CRR mechanism.

The CRR models used at present in calculations are one-electron models. The most reliable methods for calculating the response of an atom to a strong field of a light pulse are based on the direct numerical integration of the Schrödinger equation of a one-electron atom in an oscillating field. Due to the complexity of such calculations, it is difficult to use them for studying generation in a macroscopic medium. At the same time, in the case of a one-electron atom, the numerical integration of the Schrödinger equation makes it possible to calculate the response with high accuracy and can be used, in particular, to test less accurate but also less complex calculation models.

The high-frequency response of an atom to a strong excitation is calculated in the majority of modern papers by using the Lewenstein model [5], in which the Schrödinger equation is solved in fact by the method of successive approximations by using the first approximation. A considerable part of calculations in this model can be performed analytically. Remaining comparatively cumbersome, this

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model, nevertheless, is often used to calculate generation in macroscopic media. The model has given a number of correct qualitative conclusions about the dependence of the atomic response on various parameters; however, the response amplitude predicted by this model is significantly lower than that calculated numerically from the Schrödinger equation.

In [6], a comparatively simple algorithm based on the semiclassical theory was developed for calculations of the atomic response to an intense periodic field. Thus, it was demonstrated that the methods and assumptions of the semiclassical theory can be used not only for the qualitative interpretation but also for quantitative calculations of the response of a medium to the wave field. This algorithm used the spectral representation and can be used to describe HOHG in the field of a rather long pulse. It employs in the explicit form the assumption about the periodicity of the process and, hence, about the discrete structure of the generated emission spectrum. The spectrum of an atomic response to a short pulse is almost continuous. In this case, it is more convenient to calculate the response in the time representation.

In this paper, we developed an algorithm based on the semiclassical CRR theory and derived expressions for calculations (in the time representation) of the atomic response to the field of a linearly polarised light pulse of an arbitrary duration. These expressions were tested by calculating the response by integrating numerically the Schrödinger equation for a hydrogen atom and comparing the result with results obtained by using this algorithm. Strictly speaking, the proposed calculation algorithm is based on the assumption about the tunnel ionisation mechanism. The tests showed that it can be used in a broader range of exciting light intensities including the region of multiphoton and above-barrier ionisation.

Below, we discuss the algorithm for calculating any atoms treated as a one-electron atom. Then, general expressions are written in a specific form for the hydrogen atom. The method of numerical integration of the Schrödinger equation for the hydrogen atom is briefly discussed and the results of calculations of the atomic response obtained by numerical integration and by using the proposed algorithm are compared.

2. The theoretical model

The high-frequency response of an atom is treated in our model as the quantum-state-averaged force $-\nabla V$ acting on an electron from an ion (V is the potential produced by the ion). The wave function of the electron is represented as a superposition of the ground-state wave function Ψ_0 and the free wave packet $\delta\Psi$. It is assumed that the term $\langle\delta\Psi|-\nabla V|\delta\Psi\rangle$ in the expression for the average force can be neglected and the quantity $\langle\Psi_0|-\nabla V|\Psi_0\rangle$ is identically zero, so that the average force can be calculated from the expression

$$f(t) = \langle\Psi_0|-\nabla V|\delta\Psi\rangle + \text{c. c.} \quad (1)$$

The expression for the ground-state wave function has the form

$$\Psi_0(t, r) = \sqrt{N_0(t)}\varphi_0(r) \exp\left(\frac{i}{\hbar}It\right), \quad (2)$$

where φ_0 is the eigenfunction of the atomic Hamiltonian; I is the ionisation potential of the atom;

$$N_0(t) = \exp\left[-\int_{-\infty}^t w(\tau)d\tau\right] \quad (3)$$

is the state population; and w is the ionisation probability. It is assumed that this probability is an instant function of the electric field strength E :

$$w(t) = W(E(t)). \quad (4)$$

The assumption about the instant ionisation in the semiclassical CRR theory is principal. In particular, it is used in the construction of the wave packet of a free electron.

Because the ground state is localised within a small spatial region, only a small part of the wave packet $\delta\Psi$ near the ion makes a considerable contribution to force (1). Therefore, the wave packet should be described only in this region. It can be represented here as a sum of plane quasi-classical packets of the form

$$\varphi(t, x) = \sqrt{\rho(t)} \exp\left[\frac{i}{\hbar}S(t, x)\right], \quad (5)$$

where ρ is the wave-packet density; S is the action; and x is the coordinate along the linearly polarised exciting field E . The structure of functions (5) is determined based on the following considerations related to the assumption about the instant nature of ionisation and recombination. At the instant of time t , an electron flies by a nucleus, which has tunneled at the instant t_{ion} to the point $x_{\text{ion}}(E(t))$. It is assumed that the values of ρ and S in (5) are determined by the trajectory and time of the free flight of this electron, which are calculated by using classical equations of motion (see below). The time $t_{\text{ion}}(t)$ is calculated simultaneously. In fact, the calculation of dependences $t_{\text{ion}}(t)$ is the main time-consuming calculation stage requiring the use of numerical methods. The calculations are performed by using the following assumptions.

The electron motion is described by the Newton equation

$$\frac{d^2x}{dt'^2} = -\frac{e}{m}E(t'), \quad (6)$$

where $t' \in [t_{\text{ion}}, t]$. Immediately after ionisation [at the instant $t_{\text{ion}}(t)$], the electron is at rest, i.e.

$$\dot{x}(t_{\text{ion}}) = 0, \quad (7)$$

and is located at the point x_{ion} depending on the instant value of the field strength:

$$x(t_{\text{ion}}) = x_{\text{ion}}(E(t_{\text{ion}})); \quad (8)$$

the electron motion ends near the parent ion, i.e.

$$x(t) = 0. \quad (9)$$

By integrating twice Eqn (6) and substituting conditions (7)–(9) into the obtained expression, we obtain the equation

$$\frac{mc}{e}x_{\text{ion}}(t_{\text{ion}}) + \int_{t_{\text{ion}}}^t A(\tau)d\tau - (t - t_{\text{ion}})A(t_{\text{ion}}) = 0 \quad (10)$$

relating t_{ion} and t , where $A(\tau)$ is the vector potential. The tunnelling coordinate x_{ion} (8) can be determined from the equation

$$-eV(x_{\text{ion}}) - eE(t_{\text{ion}})x_{\text{ion}} = -I. \quad (11)$$

The pair of instants of time (t_{ion}, t) representing the solution of Eqn (10) determines unambiguously one of the possible electron trajectories $x(t')$. It is important to note that Eqn (10) has several roots $t_{\text{ion}}(t)$ in the general case for fixed t , i.e. there exist several ionisation moments corresponding to one recombination moment. This is related to the presence of oscillations in the dependence $E(t')$. In final expression (1) for the force, it is necessary to add the contributions from all possible recombining electrons whose trajectories are determined by the many-valued dependence $t_{\text{ion}}(t)$. Meanwhile, we assume that the wave packet of a free electron contains only one term of type (5) corresponding to one of the roots $t_{\text{ion}}(t)$. Thus, the wave packet of a free electron is represented in the form

$$\delta\Psi(t, x) = \varphi(t, x).$$

The action S is calculated from the expression

$$S(t, x) = It_{\text{ion}} - \int_{t_{\text{ion}}}^t \frac{p_x^2(\tau)}{2m} d\tau + (x - x_{\text{ion}})p_x, \quad (12)$$

where p_x is the mechanical momentum of a free electron. An arbitrary constant in (12) is selected so that the phases of the wave packet $\delta\Psi$ and ground-state wave function Ψ_0 would coincide at the ionisation moment at the point $x = x_{\text{ion}}$.

The density ρ of the wave packet of a free electron can be estimated as the ratio of the number of electrons ionised during the time interval δt_{ion} to the volume containing these electrons at the corresponding recombination moment. This volume is equal to the product of the wave-packet cross section S_{\perp} (defined below) by the distance propagated by the packet at the velocity p_x/m for the time $\delta t = |dt/dt_{\text{ion}}|\delta t_{\text{ion}}$. As a result, we obtain

$$\rho = \frac{N_0(t_{\text{ion}})w(t_{\text{ion}})\delta t_{\text{ion}}}{(p_x/m)\delta t S_{\perp}} = \frac{N_0(t_{\text{ion}})mw(t_{\text{ion}})}{S_{\perp}p_x} \left| \frac{dt_{\text{ion}}}{dt} \right|. \quad (13)$$

The electron momentum p_x can be found from the law of conservation of canonical momentum. Then,

$$p_x(t) = \frac{e}{c}[A(t) - A(t_{\text{ion}})]. \quad (14)$$

The derivative dt_{ion}/dt can be determined from Eqn (10). By using the rule for differentiating implicit functions, we obtain

$$\frac{dt_{\text{ion}}}{dt} = \frac{A(t) - A(t_{\text{ion}})}{(t - t_{\text{ion}})\dot{A}(t_{\text{ion}}) - (mc/e)\dot{x}_{\text{ion}}(t_{\text{ion}})}. \quad (15)$$

The wave-packet cross section S_{\perp} can be estimated as follows. Because the free flight time $t - t_{\text{ion}}$ is large, as a

rule, the electron wave packet strongly spreads during free motion. Its cross section S_{\perp} is mainly determined by the dispersion of the transverse component of the momentum, while the initial size of the electron can be neglected. Then, we have $S_{\perp} \approx K\pi(p_{\perp}^2/m^2)(t - t_{\text{ion}})^2$, where p_{\perp}^2 is the dispersion of the transverse component of the momentum after ionisation.

The momentum dispersion in the tunnel ionisation regime is described by the expression [7] $p_{\perp}^2 = 2mIE/E_0$, where $E_0 = (e/r_{\text{B}}^2)(I/Ry)^{1/2}$ is the intraatomic field and r_{B} is the Bohr radius in the hydrogen atom. By using this result, we can represent the expression for the cross section of the electron wave packet flying up to the parent ion in the form

$$S_{\perp} \approx K\pi r_{\text{B}}^2 \frac{2E(t_{\text{ion}})I}{me} (t - t_{\text{ion}})^2 \left(\frac{Ry}{I} \right)^{1/2}, \quad (16)$$

where K is the dimensionless coefficient which is obtained from the following considerations. The ratio $S_{\perp}/(\pi r_{\text{B}}^2)$ is always large, i.e. a free wave packet strongly spreads. It is natural to assume that Coulomb forces cause some contraction of the wave packet to the axis, which is not necessarily uniform and is especially significant for small values of the momentum p_x when the electron slowly passes through the force centre region. This contraction can be treated as scattering by a Coulomb centre. Therefore, we introduce the correcting factor K in the form [6]

$$K(p_x) = \frac{\pi r_{\text{B}}^2}{\pi r_{\text{B}}^2 + S_{\text{sc}}(p_x)}, \quad (17)$$

where $S_{\text{sc}}(p_x) = 16\pi r_{\text{B}}^2 m^2 I^2 / p_x^4$ is the cross section of scattering of a classical electron with the momentum p_x by angles exceeding $\pi/2$.

By substituting (2), (5), and (12) into (1), we obtain the expression for the force

$$f(t) \approx -a(t) \exp[-i\Phi(t)] + \text{c. c.}, \quad (18)$$

where

$$a(t) = \langle \varphi_0 | -\nabla V | \exp(-ip_x x/\hbar) \rangle (N_0 \rho)^{1/2}; \quad (19)$$

$$\Phi(t) = \frac{1}{\hbar} \left[I(t - t_{\text{ion}}) + \int_{t_{\text{ion}}}^t \frac{p_x^2(\tau)}{2m} d\tau + x_{\text{ion}} p_x(t) \right]. \quad (20)$$

2.1 Hydrogen atom

The expressions presented above were written for an arbitrary atom. To obtain the closed system of formulas and equations, it is necessary to specify the form of the potential produced by the ion, ionisation probabilities (4), and the ground-state wave function Ψ_0 . This procedure is performed below for the hydrogen atom.

In this case, we have $(-\nabla V)_x = -e^2 x/r^3$. Equation (11) has the solution

$$x_{\text{ion}}(t_{\text{ion}}) = \frac{I}{2eE(t_{\text{ion}})} + \left\{ \left[\frac{I}{2eE(t_{\text{ion}})} \right]^2 - \frac{e}{E(t_{\text{ion}})} \right\}^{1/2}. \quad (21)$$

For $E(t_{\text{ion}}) > I^2/(4e^3)$, the radicand in (21) is negative (above-barrier ionisation occurs). In this case, we calculate the tunnelling coordinate from the expression

$$x_{\text{ion}}(t_{\text{ion}}) = \frac{I}{2eE(t_{\text{ion}})}. \quad (22)$$

The ionisation probability for the hydrogen atom is calculated from the expression [8]

$$W_{\text{H}}(E) = \frac{2I4E_0}{\hbar E} \exp\left(\frac{-2E_0}{3E}\right). \quad (23)$$

We write relation (4) by replacing the argument t in its right-hand side by $t - \hbar/I$ (the expediency of this replacement was discussed in [6]):

$$w_{\text{H}}(t) = W_{\text{H}}(E(t - \hbar/I)). \quad (24)$$

By substituting the function φ_0 , corresponding to the ground state of the hydrogen atom, to expression (19), we obtain

$$a_{\text{H}} = 8iIG \left(\frac{p_x}{p_0} \right) (\pi r_{\text{B}} N_0 \rho)^{1/2}, \quad (25)$$

where

$$G(\xi) = \frac{\xi - \arctan \xi}{\xi^2}; \quad p_0 = \sqrt{2mI}.$$

Thus, the force exerted by the ion on the electron in the hydrogen atom can be analytically calculated by expressions (18)–(20) taking into account expressions (3), (13)–(16) (20), (21)–(25) and dependences $t_{\text{ion}}(t)$ obtained by solving numerically Eqn (10). The contributions from all the roots $t_{\text{ion}}(t)$ in final expression (18) should be summed. Note that the primitive from $A(t)$ in (10) can be found either analytically or tabulated preliminary. Therefore, Eqn (10) can be considered as an algebraic equation. We solved this equation by using a simple but rather efficient algorithm described in Appendix.

As a whole, the algorithm for calculation of the atomic response involves the following stages:

(i) The vector-potential A of the electric field, the momentum and the square of momentum (14) of a free electron, and their primitives and the population $N_0(t)$ are tabulated or calculated analytically.

(ii) Equation (10) is solved for all possible values of t .

(iii) The ionisation probability $W(E(t_{\text{ion}}))$, the tunnelling coordinate $x_{\text{ion}}(t_{\text{ion}}(t))$, the cross section S_{\perp} , and the wave-packet density ρ , which are the functions of the current time t , are calculated by expressions (23), (24), (21), (22), (16), (17), (13), and (15) for each solution of Eqn (10).

(iv) The phase Φ and amplitude a_{H} of the force acting on the electron are calculated by expressions (20) and (25) for each solution of Eqn (10).

(v) The dependence $f(t)$ is calculated by expression (18) and the contributions of all the roots $t_{\text{ion}}(t)$ of Eqn (10) are summarised. In fact, the main contribution to CRR is introduced by electrons that are free during the time shorter than the field period. We performed a number of calculations by neglecting free electrons recombining after ionisation for the time exceeding the field period. In the region of low frequencies (close to I/\hbar), the results of such calculations only slightly differed from the results of calculations taking into account all free electrons, while in the high-frequency region these results completely coincided.

Although the analysis performed above concerned a one-electron atom, it can be also applied for many-electron atoms by using model potentials. It is important in this connection that only the ionisation probability, the ion potential $V(r)$, and the ground-state wave function Ψ_0 strongly depend on the properties of a particular atom in the expressions obtained. The ionisation probability in the tunnelling regime was considered in [9] and other papers. Potentials produced by various ions were studied in [10]. By using the results of these papers, we can apply the theory developed here to the case of many-electron atoms.

3. Calculation of the response by integrating numerically the Schrödinger equation

We tested the described algorithm by performing a number of calculations of the quantity

$$f_{\text{num}}(t) = \langle \Psi | -\nabla V | \Psi \rangle, \quad (26)$$

in which the wave function Ψ was found by integrating numerically the Schrödinger equation

$$i\hbar\dot{\Psi} = \left[\frac{\hat{p}^2}{2m} - \frac{e^2}{r} + exE(t) \right] \Psi$$

for the hydrogen atom, where E is the electric field of a linearly polarised light pulse. We used the method of numerical integration discussed in [11]. The calculations were performed in cylindrical coordinates on a network with variable steps. To avoid reflections from boundaries, we used continuously switching absorbers. The size and maximum steps of a spatial network and parameters of absorbers were varied till it affected the results obtained.

4. Discussion of results and conclusions

Test calculations were performed by using a cosine pulse of duration two and a half periods at a wavelength of $1.06 \mu\text{m}$ shown in Fig. 1, where the time dependence of the total force acting on an electron is also presented.

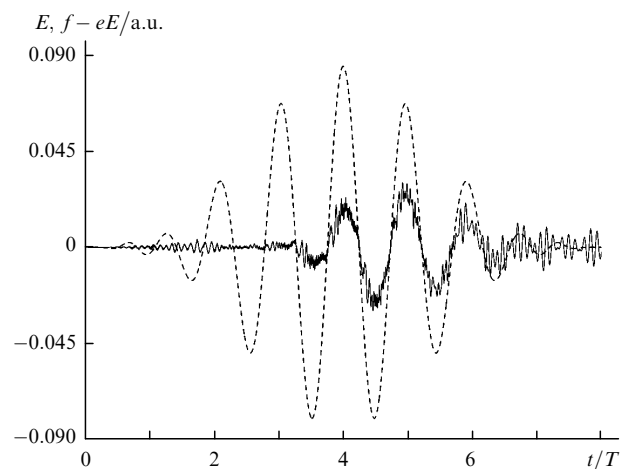


Figure 1. Electric field strength $E(t)$ of the exciting wave (dashed curve) and the total force $f(t) - eE(t)$ acting on an electron (solid curve) as functions of time (in field periods T).

Figure 2 demonstrates the spectra of forces (1) and (26) calculated by expressions derived in our model and obtained by the numerical integration of the Schrödinger equation for the peak power of the exciting pulse equal to $2.5 \times 10^{14} \text{ W cm}^{-2}$. (Because the semiclassical theory is valid only for radiation with frequencies $\omega > I/\hbar$, only this spectral region is shown.) In the high-frequency region, good agreement between the cut-off frequencies and squares of the Fourier transforms $f_\omega(\omega)$ of the force obtained by these two methods is observed.

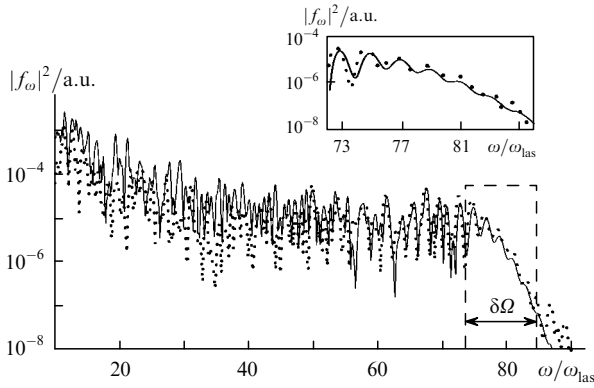


Figure 2. Frequency dependences of the square $|f_\omega|^2$ of the Fourier transform of the force acting on an electron obtained by solving numerically the Schrödinger equation (solid curve) and from model expressions (dashed curve); ω_{las} is the carrier excitation frequency.

Note in this connection that the separation of a single AP from the total radiation field is reduced to the separation of a narrow frequency interval adjacent to the cut-off frequency from the total generated spectrum. Radiation at such frequencies is generated at the end of the half-period where the electric field of the exciting wave is maximal [12] (Fig. 3). For this reason, the coincidence of spectra (1) and (26) in the cut-off frequency region provides the coincidence of separated APs.

The spectral filtration was performed by the expression

$$f_{\text{fil}}(t) = \frac{1}{\sqrt{2\pi}} \int_{\delta\Omega} f_\omega(\omega) \exp(-i\omega t) d\omega, \quad (27)$$

where $\delta\Omega$ is the frequency interval shown in Fig. 2. Figure 3 presents the squares of the modulus of force (27) calculated by using spectra shown in Fig. 2. One can see that APs obtained by spectral filtration are close to each other in duration, amplitude, and spectral filling, and are generated at the same instant of time.

Other spectral regions lying within the plateau in Fig. 2 can be separated similarly. (As the frequency interval $\delta\Omega$ is shifted inside the plateau, the contrast of produced APs decreases.) The results obtained by the two methods virtually coincide if the interval $\delta\Omega$ is located to the right of the plateau centre in Fig. 2.

The laser radiation intensity used in calculations presented in Fig. 2 corresponds to the region of above-barrier ionisation (this region begins formally at the intensity of $1.4 \times 10^{14} \text{ W cm}^{-2}$). Test calculations showed that our model provides good agreement with the results of numerical integration of the Schrödinger equation in the intensity

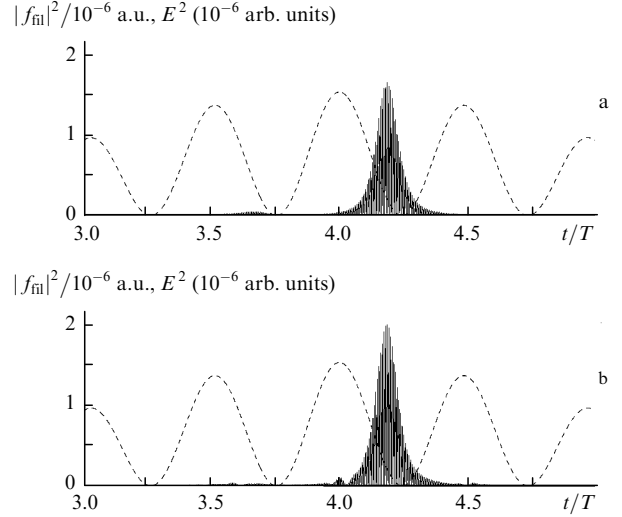


Figure 3. Dependences of the square $|f_{\text{fil}}|^2$ of the spectrally filtered force (solid curve) and the square E^2 of the electric field of the exciting pulse (dashed curve) on time (in field periods T) obtained from model expressions (a) and by solving numerically the Schrödinger equation (b).

range $(0.7 - 3.5) \times 10^{14} \text{ W cm}^{-2}$ (in this range, the AP durations calculated by the two methods virtually coincide, while their amplitudes differ by less than 30%). The Keldysh parameter at the lower boundary of this region is close to unity, so that we can assume that here ionisation already occurs by tunnelling. However, a greater part of the above-mentioned intensity range lies in the region corresponding formally to above-barrier ionisation. It seems that basic assumptions used in the semiclassical model are also valid in the case of the above-barrier ionisation of atoms.

Note that for intensities exceeding $3.5 \times 10^{14} \text{ W cm}^{-2}$, the generation of coherent high-frequency radiation is less efficient [11], so that this range is the most interesting for generating APs.

Thus, the algorithm based on the semiclassical CRR model developed in the paper allows one to calculate quite accurately the response of a one-electron atom to the field of a linearly polarised laser pulse of duration of a few optical field cycles. The results of model calculations well agree with the numerical solution of the Schrödinger equation. The calculation complexity of the algorithm is two and more orders of magnitude lower than that of any algorithm of the numerical integration of the two-dimensional Schrödinger equation on a network for the parameters of the exciting pulse typical for experiments on generating APs.

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Appendix

The algorithm for calculating CRR formulated above contains only one complex calculation stage, namely, the solution of algebraic equation (10). The current time t (recombination instant) in this equation is assumed specified, whereas the ionisation instant t_{ion} is unknown. Equation (10) can be formally written as

$$F(t_{\text{ion}}, b)|_{b=t} = 0. \quad (A1)$$

Equation (A1) is solved by N times for the values $b_k = k\Delta t$, where $k = 1, 2, \dots, N$, and Δt is the time step which is related to the maximum frequency of radiation generated during CRR as $\Delta t < \pi/\omega_{\max}$. The number of steps N should be sufficient for the product $N\Delta t$ to exceed the exciting pulse duration.

The results of calculations of the CRR parameters in the hydrogen atom almost do not change when Eqn (A1) is solved with the error exceeding Δt . Thus, there is no need to calculate t_{ion} with a higher accuracy, and therefore all the roots $t_{\text{ion}}(a_k)$ also can be considered multiple of Δt and represented in the form $t_{\text{ion}}(b_k) = m\Delta t$, where m is an integer.

It is important that the function $F(t_{\text{ion}}b_k)$ is continuous everywhere except points in which the electric field is zero. By using this property, we can assert that solutions $m\Delta t$ satisfy the condition

$$F(\Delta t m, b_k)F(\Delta t (m + 1), b_k) \leq 0. \quad (\text{A2})$$

Therefore, we can seek the roots of Eqn (A1) by verifying the validity of inequality (A2) for all values $m < k$. The roots lie at the points where the inequality is fulfilled. Solutions related to the zero electric field can be discarded after calculating all the values of m satisfying inequality (A2) for fixed k .

This algorithm for solving Eqn (A2) does not pretend to be optimal but it allows one to find all the solutions of the equation with certain accuracy. In addition, the structure of Eqn (10) and inequality (A2) makes it possible to realise efficiently this algorithm in modern computers without the explicit verification of the conditional operator.

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